Ana Sofia Oliveira

List of Publications by Year
in descending order

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27	744	567144 15	552653 26
papers	citations	h-index	g-index

36	36	36	1004
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The fatty acid site is coupled to functional motifs in the SARS-CoV-2 spike protein and modulates spike allosteric behaviour. Computational and Structural Biotechnology Journal, 2022, 20, 139-147.	1.9	19
2	Structural insights in cell-type specific evolution of intra-host diversity by SARS-CoV-2. Nature Communications, 2022, 13, 222.	5.8	23
3	Rate-limiting transport of positively charged arginine residues through the Sec-machinery is integral to the mechanism of protein secretion. ELife, 2022, 11, .	2.8	13
4	Identification and validation of novel microtubule suppressors with an imidazopyridine scaffold through structure-based virtual screening and docking. RSC Medicinal Chemistry, 2022, 13, 929-943.	1.7	6
5	A conserved arginine with nonâ€conserved function is a key determinant of agonist selectivity in Î±7 nicotinic ACh receptors. British Journal of Pharmacology, 2021, 178, 1651-1668.	2.7	6
6	A potential interaction between the SARS-CoV-2 spike protein and nicotinic acetylcholine receptors. Biophysical Journal, 2021, 120, 983-993.	0.2	43
7	ATP hydrolysis and nucleotide exit enhance maltose translocation in the MalFGK2E importer. Scientific Reports, 2021, 11, 10591.	1.6	1
8	Dynamical nonequilibrium molecular dynamics reveals the structural basis for allostery and signal propagation in biomolecular systems. European Physical Journal B, 2021, 94, 144.	0.6	23
9	Molecular dynamics simulations support the hypothesis that the brGDGT paleothermometer is based on homeoviscous adaptation. Geochimica Et Cosmochimica Acta, 2021, 312, 44-56.	1.6	28
10	Resistance to the â€œlast resortâ€•antibiotic colistin: a single-zinc mechanism for phosphointermediate formation in MCR enzymes. Chemical Communications, 2020, 56, 6874-6877.	2.2	10
11	Identification of the Initial Steps in Signal Transduction in the Î±4Î²2 Nicotinic Receptor: Insights from Equilibrium and Nonequilibrium Simulations. Structure, 2019, 27, 1171-1183.e3.	1.6	24
12	Regulation of the mechanism of Type-II NADH: Quinone oxidoreductase from S. aureus. Redox Biology, 2018, 16, 209-214.	3.9	18
13	Unlocking Nicotinic Selectivity via Direct Câ€'H Functionalization of (â^')-Cytisine. CheM, 2018, 4, 1710-1725.	5.8	31
14	Effect of a pH Gradient on the Protonation States of Cytochrome c Oxidase: A Continuum Electrostatics Study. Journal of Chemical Information and Modeling, 2017, 57, 256-266.	2.5	5
15	Structural and Functional insights into the catalytic mechanism of the Type II NADH:quinone oxidoreductase family. Scientific Reports, 2017, 7, 42303.	1.6	22
16	Molecular structure of FoxE, the putative iron oxidase of Rhodobacter ferrooxidans SW2. Biochimica Et Biophysica Acta - Bioenergetics, 2017, 1858, 847-853.	0.5	10
17	The key role of glutamate 172 in the mechanism of type II NADH:quinone oxidoreductase of Staphylococcus aureus. Biochimica Et Biophysica Acta - Bioenergetics, 2017, 1858, 823-832.	0.5	17
18	Coupling between protonation and conformation in cytochrome c oxidase: Insights from constant-pH MD simulations. Biochimica Et Biophysica Acta - Bioenergetics, 2016, 1857, 759-771.	0.5	20

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19	Exploring O2 Diffusion in A-Type Cytochrome c Oxidases: Molecular Dynamics Simulations Uncover Two Alternative Channels towards the Binuclear Site. PLoS Computational Biology, 2014, 10, e1004010.	1.5	22
20	The Role of Lys147 in the Interaction between MPSA-Gold Nanoparticles and the Î±-Hemolysin Nanopore. Langmuir, 2012, 28, 15643-15650.	1.6	18
21	Conformational changes induced by ATPâ€hydrolysis in an ABC transporter: A molecular dynamics study of the Sav1866 exporter. Proteins: Structure, Function and Bioinformatics, 2011, 79, 1977-1990.	1.5	59
22	Structural consequences of ATP hydrolysis on the ABC transporter NBD dimer: Molecular dynamics studies of HlyB. Protein Science, 2011, 20, 1220-1230.	3.1	43
23	Inter-domain Communication Mechanisms in an ABC Importer: A Molecular Dynamics Study of the MalFGK2E Complex. PLoS Computational Biology, 2011, 7, e1002128.	1.5	28
24	Insights into the Molecular Mechanism of an ABC Transporter: Conformational Changes in the NBD Dimer of MJ0796. Journal of Physical Chemistry B, 2010, 114, 5486-5496.	1.2	31
25	Hydrogenases in Desulfovibrio vulgaris Hildenborough: structural and physiologic characterisation of the membrane-bound [NiFeSe] hydrogenase. Journal of Biological Inorganic Chemistry, 2005, 10, 667-682.	1.1	83
26	On the Use of Different Dielectric Constants for Computing Individual and Pairwise Terms in Poissonâ^'Boltzmann Studies of Protein Ionization Equilibrium. Journal of Physical Chemistry B, 2005, 109, 14691-14706.	1.2	91
27	Reorganization and Conformational Changes in the Reduction of Tetraheme Cytochromes. Biophysical Journal, 2005, 89, 3919-3930.	0.2	22